An optimal Vlasov-Fokker-Planck solver for simulation of kinetic ICF plasmas

L. Chacón[1], W.T. Taitano[2], A.N. Simakov[2]

[1]T-5, Applied mathematics and plasma physics group
[2]XCP-6, plasma theory and applications group

Thermonuclear Burn Initiative

Kinetic Effects in ICF Workshop
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Outline

- Motivations and challenges of fully kinetic ion simulations
- Enabling Technologies
  - Fully implicit time stepping + scalable solver (MG precond JFNK)
  - Exact discrete conservation properties
  - Phase-space adaptivity: v_{th} adaptivity + Lagrangian mesh
- Progress report: verification, spherical geometry (shocks), kinetic effects at interfaces

Kinetic effects may be important in ICF

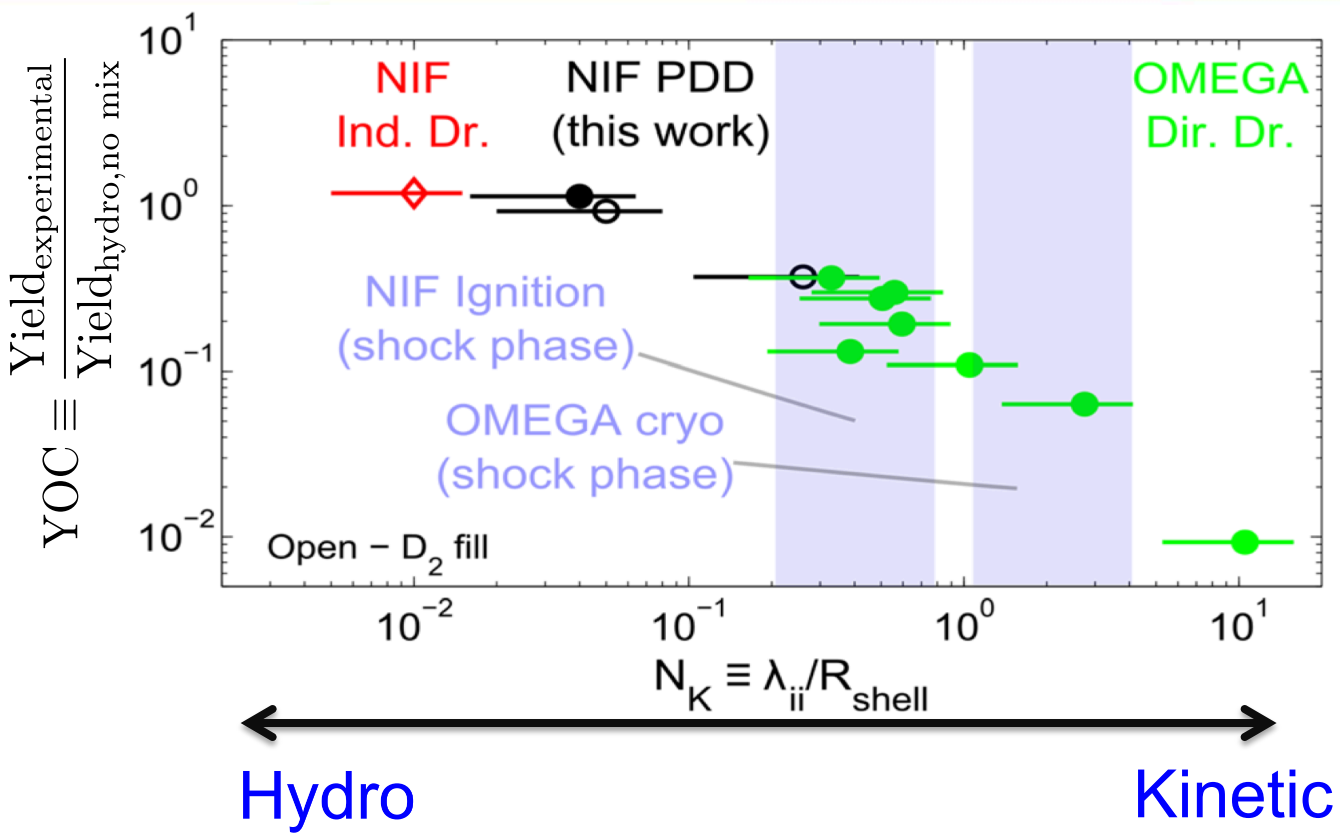


Figure from M.J. Rosenberg, PRL (2014)

We consider fully kinetic ions + fluid electrons

Vlasov-Fokker-Planck

$$\frac{Df_i}{Dt} \equiv \frac{\partial f_i}{\partial t} + \vec{v}\cdot\nabla f_i + \vec{a}_i \cdot \nabla_v f_i = \sum_j C_{ij}\left(f_i, f_j\right)$$

$$C_{ij}\left(f_i, f_j\right) = \Gamma_{ij}\nabla_v \cdot \left[\, D_j \cdot \nabla_v f_i - \frac{m_i}{m_j} A_j f_i \,\right]$$

$$D_j = \nabla_v \nabla_v G_j \qquad A_j = \nabla_v H_j$$

$$\nabla_v^2 H_j\left(\vec{v}\right) = -8\pi f_j\left(\vec{v}\right)$$

$$\nabla_v^2 G_j\left(\vec{v}\right) = H_j\left(\vec{v}\right)$$

Fluid electrons

$$\frac{3}{2}\partial_t\left(n_e T_e\right) + \frac{5}{2}\partial_x\left(u_e n_e T_e\right) - u_e \partial_x\left(n_e T_e\right) - \partial_x \kappa_e \partial_x T_e = \sum_\alpha C_{e\alpha}$$

$$n_e = -q_e^{-1}\sum^{N_s} q_\alpha n_\alpha \qquad u_e = -q_e^{-1} n_e^{-1} \sum_{\alpha\neq e}^{N_s} q_\alpha n_\alpha u_\alpha$$

Electric field model: e pressure, friction, thermal forces

$$E = -\frac{\nabla p_e + \sum_i \mathbf{F}_{ie}}{e n_e} = -\frac{\nabla p_e}{e n_e} - \frac{\alpha_0(Z_{eff}) m_e}{e}\sum_i \nu_{ei}(\mathbf{V}_e - \mathbf{V}_i) - \frac{\beta_0(Z_{eff})}{e}\nabla T_e$$

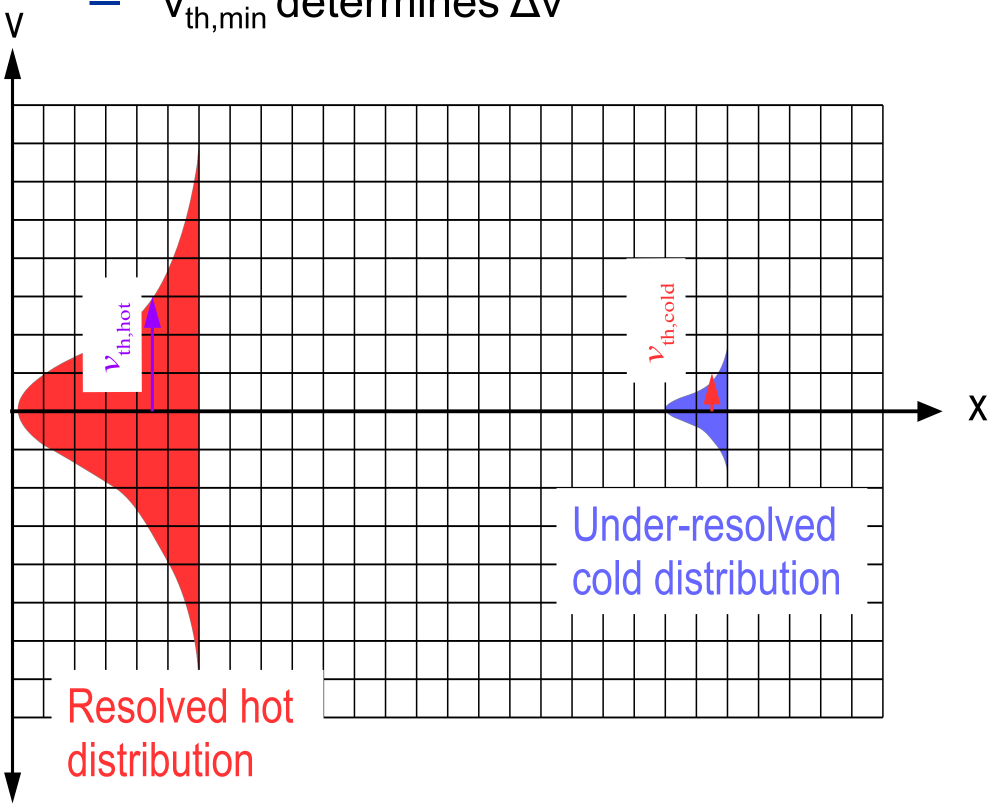
ICF kinetic simulation tools are sparse

- French CEA's FPion [1] and FUSE [2] codes:
  - Semi-implicit ($\Delta t \sim \tau_{col}$ e.g. can't study pusher mix)
  - Adaptive grid (r-v), but non-conservative, single-species velocity
- Recent implosion calculation using the LSP code [3]
  - Hybrid PIC code
  - Difficulties with spherical geometry
  - Nanbu collision operator (suspect when using $\Delta t > \tau_{col}$ [4])
- Our approach:
  - Fully nonlinearly implicit ($\Delta t >> \tau_{col}$)
  - Multispecies adaptive grid (r-v) using local thermal velocity/species
  - Fully conservative (mass, momentum, energy)

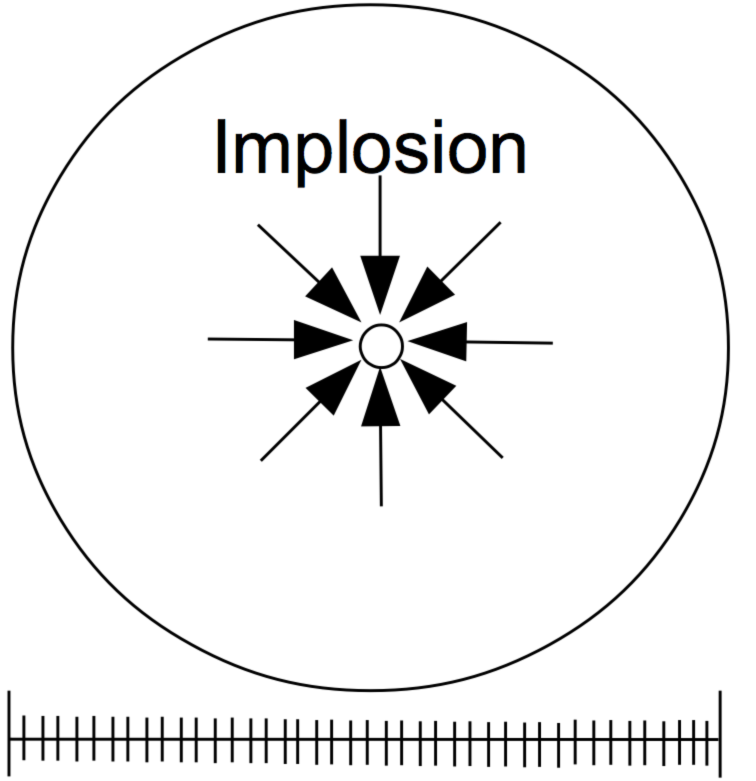
[1] O. Larroche, EPJ 27, pp.131-146 (2003)
[2] B. Peigney et al., JCP 278 (2014)
[3] T.J.T. Kwan et al., IFSA2015, Seattle WA (2015)
[4] A.M. Dimits et al., JCP 228, pp.4881-4892 (2009)

Challenges of fully kinetic simulations for ICF

- Disparate temperatures during implosion dictate velocity resolution.
  - $v_{th,max}$ determines L_v
  - $v_{th,min}$ determines Δv



- Shock width and capsule size dictate physical space resolution



Numerical resolution challenges

- Phase space resolution challenges
  - Intra species $v_{th,max} / v_{th,min} \sim 100$
  - Inter species $(v_{th,\alpha} / v_{th,\beta})_{max} \sim 30$
  - $N_v \sim [10(v_{th,max}/v_{th,min}) x (v_{th,\alpha} / v_{th,\beta})]^2 \sim 10^9$
  - $N_r \sim 10^3 - 10^4$
  - **$N = N_r N_v \sim 10^{12} - 10^{13}$ unknowns**

- Temporal resolution challenges
  - $t_{sim} = 1$ ns
  - **$N_t = 10^9$ time steps**

$$\Delta t_{exp}^{coll} \sim \frac{1}{10}\left(\frac{\Delta v}{v_{th}^{min}}\right)^2 \nu_{coll}^{-1} \sim 10^{-9}\, ns$$

Our approach: Implicit time-stepping and adaptive meshing, exact conservation properties

- Mesh adaptivity: $\hat{v} = v / v_{th,\alpha}$
  - v-space adaptivity with v_{th} normalization, $\mathbf{N_v \sim 10^4 - 10^5}$
  - Lagrangian mesh in physical space, $\mathbf{N_r \sim 10^2}$
  - $\mathbf{N = N_v N_r \sim 10^6 \sim 10^7}$
- Implicit time-stepping:
  - JFNK nonlinear solver
  - Multigrid preconditioning [1,2]
  - $\mathbf{\Delta t_{imp} = \Delta t_{str} \sim 10^{-3}}$ **ns,** $\mathbf{N_t \sim 10^3 - 10^4}$
- Exact conservation properties (nonlinear discretization)

[1] Chacon et al., JCP 157, pp. 618-653 (2000)
[2] Chacon el al., JCP 157, pp. 654-682 (2000)

Implicit time-stepping for collision operator: nonlinear solver and preconditioning

- JFNK as nonlinear solver [3]:

$$f^k = f^{k-1} - J^k R^{k-1}$$

$$R = \partial_t f_\alpha - \sum_{\beta}^{N_s} \nabla \cdot \left[\overline{\overline{D}}_\beta \cdot \nabla_v f_\alpha - \vec{A}_\beta f_\alpha \right]$$

- Right preconditioning strategy:

$$J^k \left(P^{k-1}\right)^{-1} P^{k-1} \delta f^k = -R^{k-1}$$

- Block diagonalization with lagged coefficients:

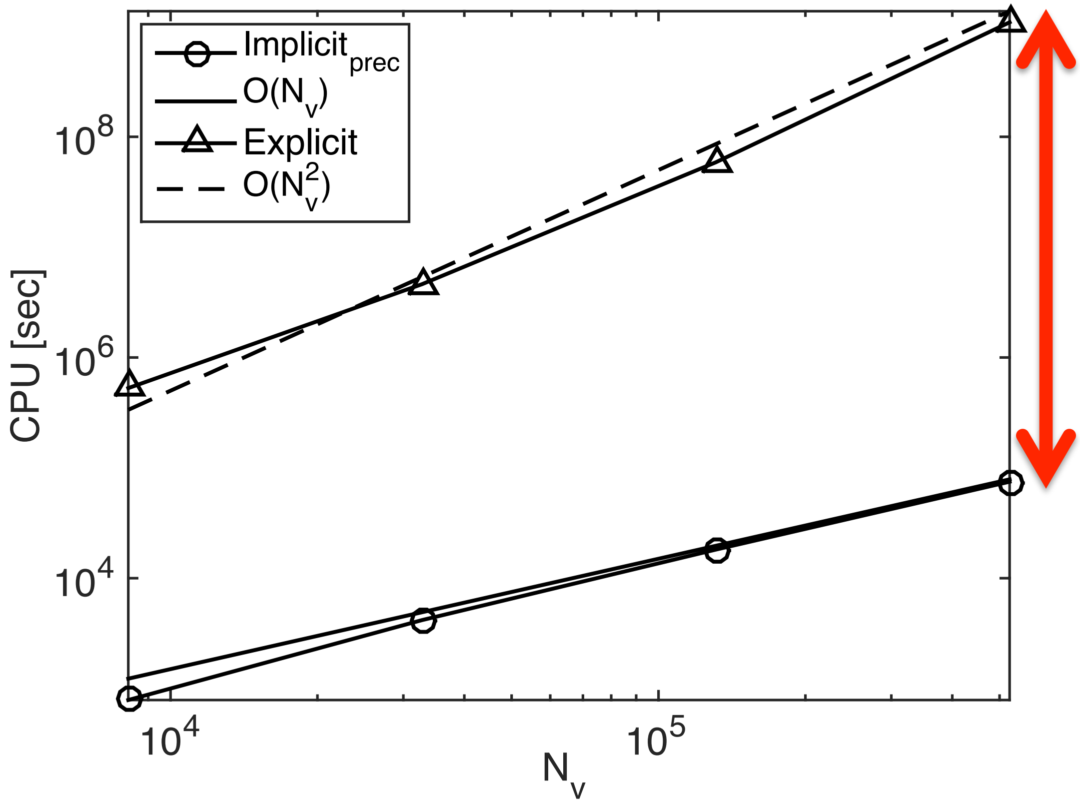
$$P^{k-1} = \partial_t \circ - \sum_{\beta}^{N_s} \nabla \cdot \left[\overline{\overline{D}}_\beta \cdot \nabla_v \circ - \vec{A}_\beta \circ \right]$$

[3] D.A. Knoll et al., JCP 193, pp. 357-397 (2004)

MG preconditioner keeps linear iterations bounded

N_v	$(\text{Preconditioned Krylov}/\Delta t)_{avg}$	$(\text{Unpreconditioned Krylov}/\Delta t)_{avg}$	$\Delta t/\Delta t_{exp}$
	$\Delta t = 10^{-3} = 2.4 \times 10^{-2}\tau_{cold}$		
128×64	2.7	3.9	6.25
256×128	2.8	7.5	28.6
512×256	2.7	12.6	122.0
	$\Delta t = 10^{-2} = 2.4 \times 10^{-1}\tau_{cold}$		
128×64	3.2	15.7	62.5
256×128	3.2	38.6	286
512×256	3.2	101.3	1220
	$\Delta t = 10^{-1} = 2.4\tau_{cold}$		
128×64	4.9	72*	625
256×128	4.3	228*	2860
512×256	4.4	783*	12 200
	$\Delta t = 10^{0} = 24\tau_{cold}$		
128×64	$8.7^\dagger$	–	6250
256×128	$7.7^\dagger$	–	28 600
512×256	$9.0^\dagger$	–	122 000

Implicit solver performance is $O(N_v)$!



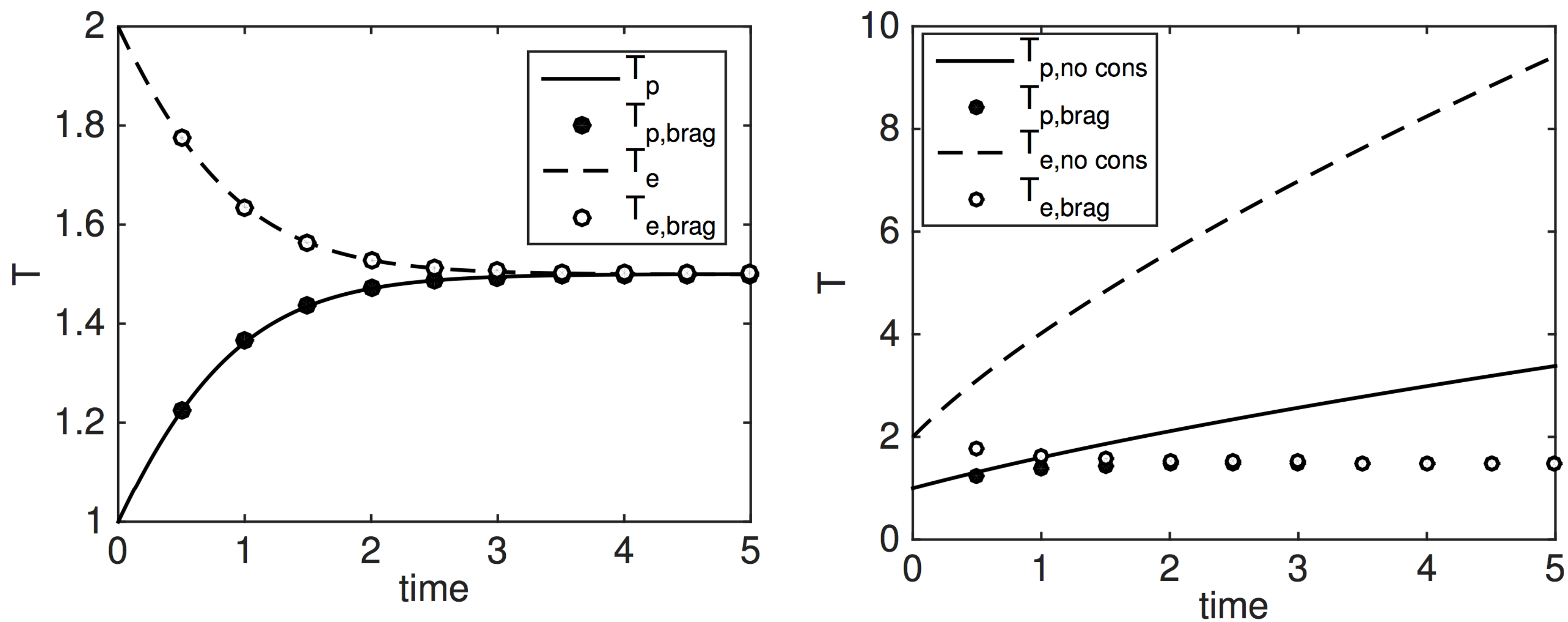
4 orders of magnitude more efficient than explicit methods

Solver CPU time versus size of unknown

[4] W.T. Taitano, JCP 297, pp.357-380 (2015)

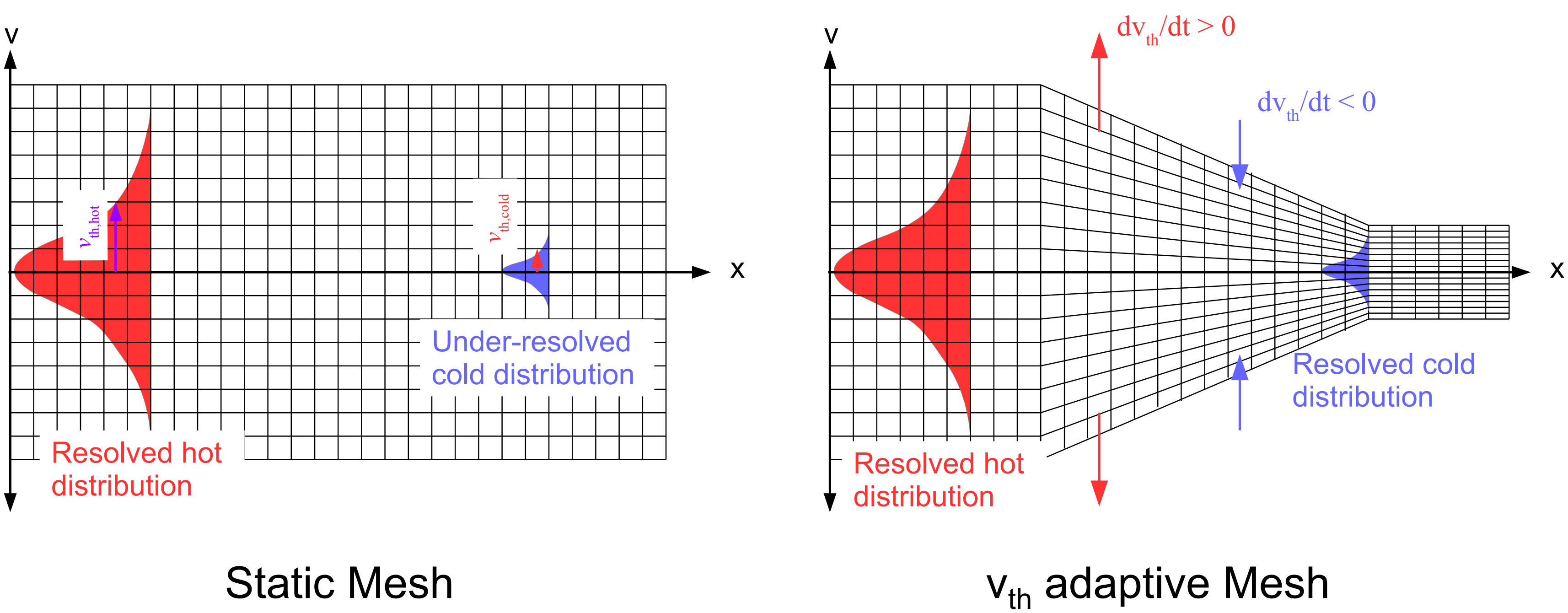
Exact energy conservation in collision operator is critical for accuracy

- For demonstration, we consider electron-proton thermalization

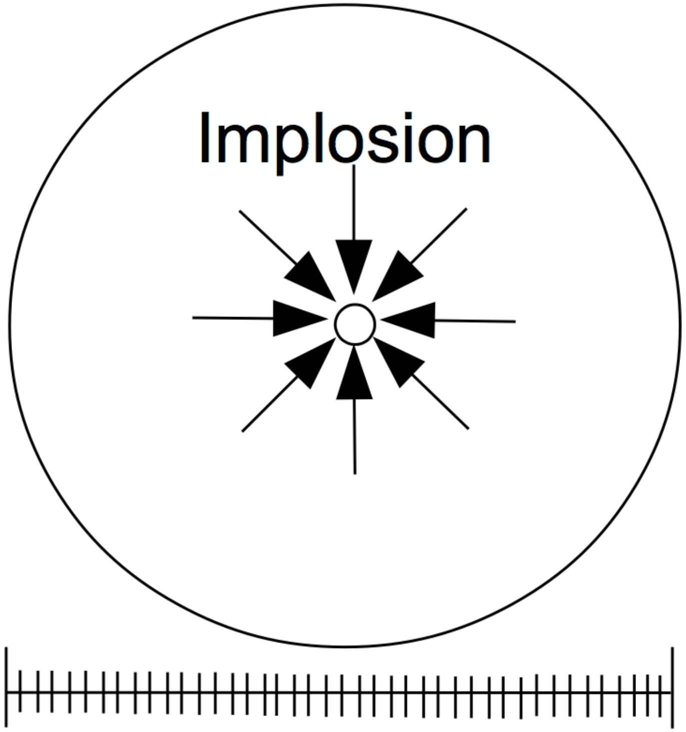


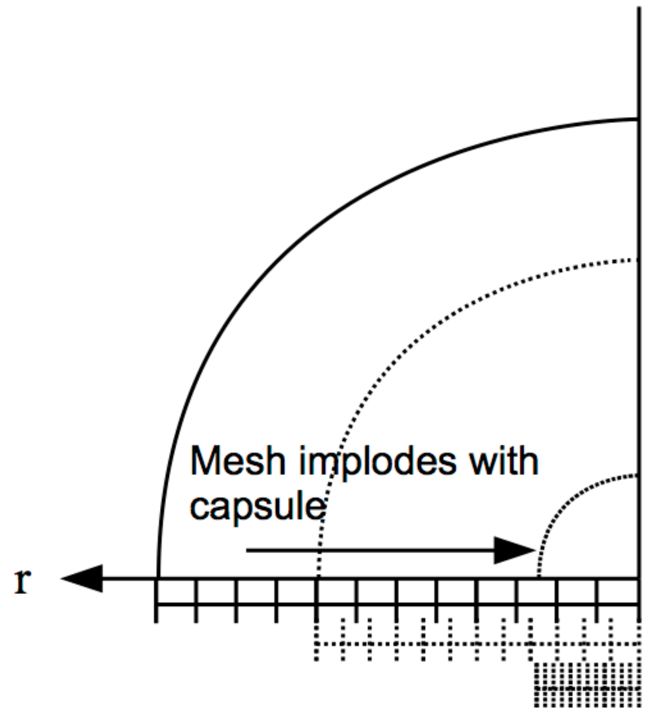
- More details in Taitano's talk

Adaptivity in velocity space: v_{th} adaptivity



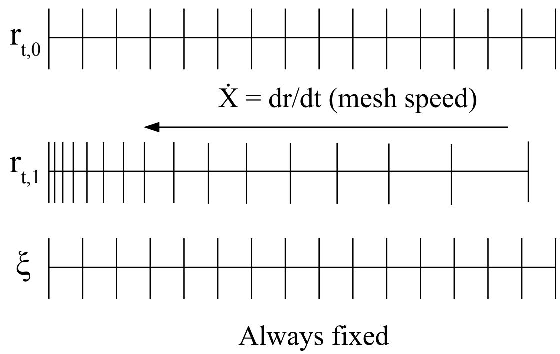
Adaptivity in physical space: Lagrangian mesh evolves with capsule

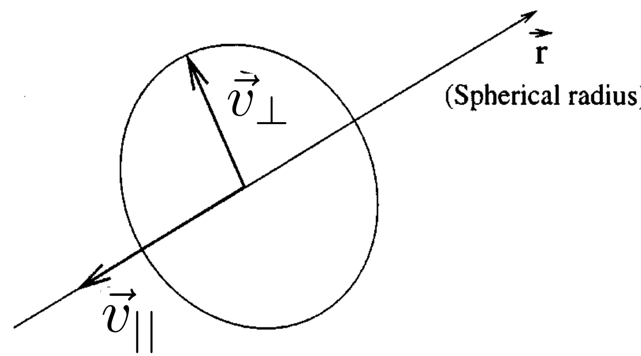




Phase-space mesh adaptivity: exact transformation of FP equation

1D spherical (with logical mesh); 2D cylindrical geometry in velocity space





Coordinate transformation:

$$\widehat{v}_{||} \equiv \frac{\vec{v} \cdot \vec{\widehat{r}}}{v_{th,\alpha}}, \quad \widehat{v}_\perp \equiv \frac{\sqrt{v^2 - v_{||}^2}}{v_{th,\alpha}}$$

Jacobian of transformation:

$$\sqrt{g_v}\,(t, r, \widehat{v}_\perp) \equiv v_{th,\alpha}^3\,(t, r)\, r^2 \widehat{v}_\perp$$

$$J_{r\xi} = \partial_\xi r$$

Fokker-Planck equation: inertial terms

- VRFP equation in transformed coordinates

$$\partial_t\left(\sqrt{g_v}J_{r\xi}f_\alpha\right)+\partial_\xi\left(\sqrt{g_v}v_{th,\alpha}\left[\widehat{v}_{||}-\boxed{\widehat{\dot{r}}_\alpha}\right]f_\alpha\right)+$$

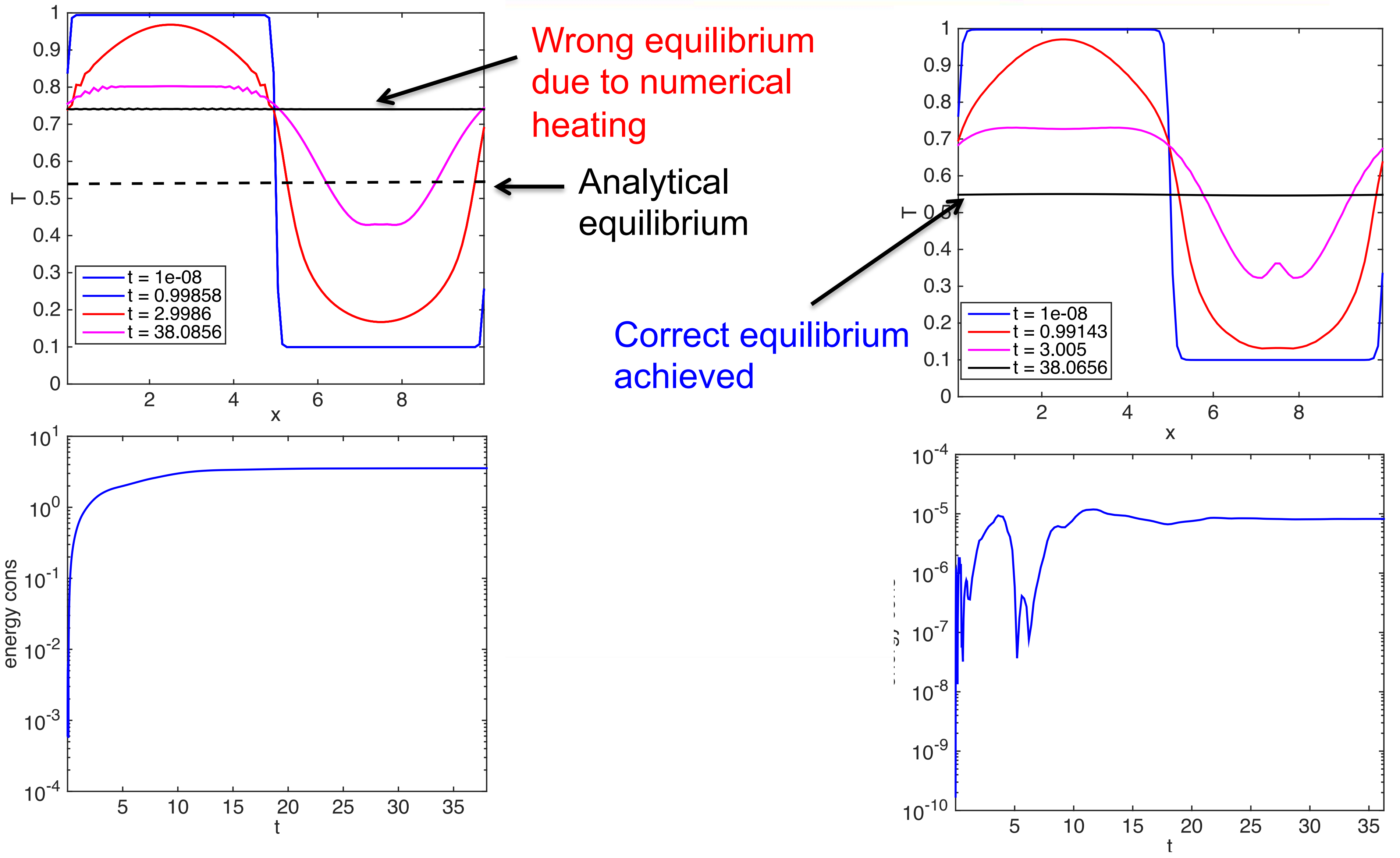
$$\partial_{\widehat{v}_{||}}\left(J_{r\xi}\sqrt{g_v}\boxed{\widehat{\dot{v}}_{||}}f_\alpha\right)+\partial_{\widehat{v}_\perp}\left(J_{r\xi}\sqrt{g_v}\boxed{\widehat{\dot{v}}_\perp}f_\alpha\right)=J_{r\xi}\sqrt{g_v}\sum_\beta^{N_s}C_{\alpha\beta}\left(f_\alpha,f_\beta\right)$$

$$\boxed{\widehat{\dot{v}}_{||}}=-\boxed{\frac{\widehat{v}_{||}}{2}\left(v_{th,\alpha}^{-2}\partial_t v_{th,\alpha}^2+J_{r\xi}^{-1}\left(\widehat{v}_{||}-\widehat{\dot{x}}\right)v_{th,\alpha}^{-1}\partial_\xi v_{th,\alpha}^2\right)}+\frac{\widehat{v}_\perp^2 v_{th,\alpha}}{r}+\frac{q_\alpha E_{||}}{J_{r\xi}m_\alpha v_{th,\alpha}}$$

$$\boxed{\widehat{\dot{v}}_\perp}=-\boxed{\frac{\widehat{v}_\perp}{2}\left(v_{th,\alpha}^{-2}\partial_t v_{th,\alpha}^2+J_{r\xi}^{-1}\left(\widehat{v}_{||}-\widehat{\dot{x}}\right)v_{th,\alpha}^{-1}\partial_\xi v_{th,\alpha}^2\right)}-\frac{\widehat{v}_{||}\widehat{v}_\perp v_{th,\alpha}}{r}$$

Inertial terms due to v_{th} adaptivity and Lagrangian mesh

Energy conservation in inertial terms is also critical for long-term accuracy



v_{th} adaptivity enables realistic simulations of multispecies plasmas

- D-e-α, 3 species thermalization problem
- Resolution with static grid:

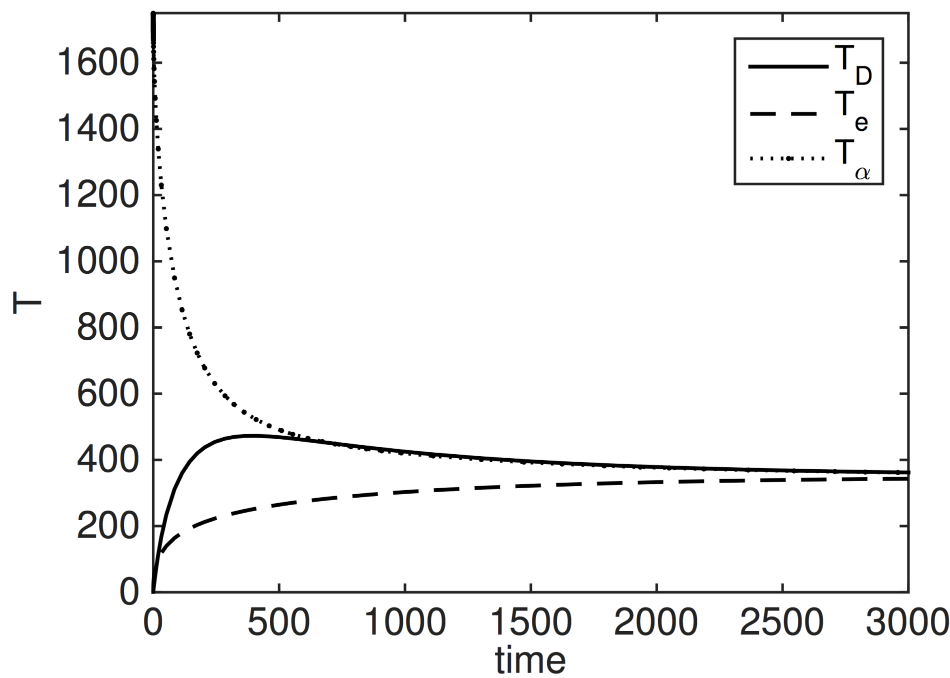
$$N_v \sim 2\left(\frac{v_{th,e,\infty}}{v_{th,D,0}}\right)^2 = 140000 \times 70000$$

- Resolution with adaptivity and asymptotics:

$$N_v = 128 \times 64$$

- **Mesh savings of**

$$\sim 10^6$$



Summary

- Developed a fully implicit, optimal Fokker-Planck solver

- Features phase-space adaptivity, optimal implicit time-stepping, and exact conservation properties
  - MG preconditioned nonlinear solver
  - Exact transformation of FP equation (no remapping)
  - Careful conservative discretization (next talk)

- As a result, we save many orders of magnitude in total simulation time

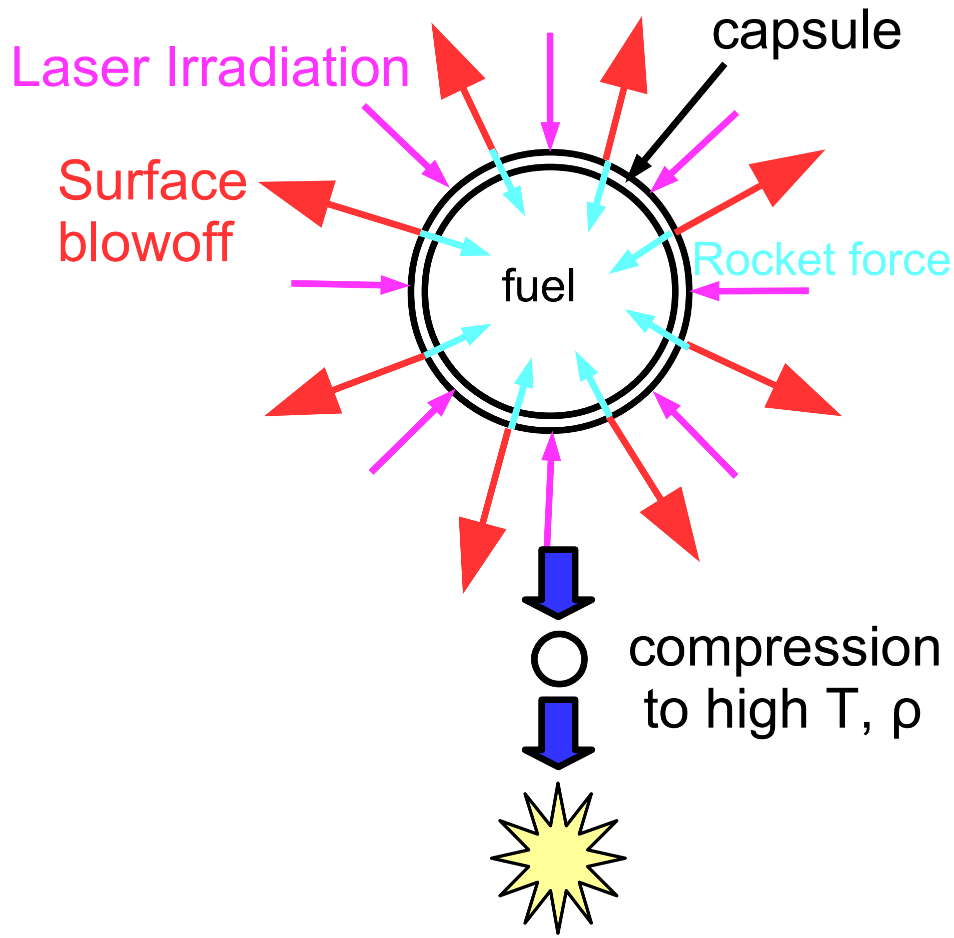
Current and Future Focus

- Both Lagrangian mesh and spherical geometry are implemented and being characterized
- Performing extensive verification campaign with shock propagation in planar and spherical geometry (next talk)
- Carry out planar geometry simulation campaign (this FY)
- Prepare for spherical ICF simulations (next FY)

BACKUP SLIDES

Questions?

How does ICF work?



Rosenbluth-Fokker-Planck collision operator: simultaneous conservation of mass, momentum, and energy

Rosenbluth-FP collision operator: conservation properties results from symmetries

$$C_{\alpha\beta} = \Gamma_{\alpha\beta} \nabla_v \cdot \left[\vec{J}_{\alpha\beta,G} - \frac{m_\alpha}{m_\beta} \vec{J}_{\alpha\beta,H} \right]$$

Mass

$$\langle 1, C_{\alpha\beta} \rangle_{\vec{v}} = 0 \quad \Rightarrow \quad \boxed{\left. \vec{J}_{\alpha\beta,G} - \vec{J}_{\alpha\beta,H} \right|_{\partial \vec{v}} = 0}$$

Momentum

$$m_\alpha \langle \vec{v}, C_{\alpha\beta} \rangle_{\vec{v}} = -m_\beta \langle \vec{v}, C_{\beta\alpha} \rangle_{\vec{v}} \quad \Rightarrow \quad \boxed{\left\langle 1, J^{\|}_{\alpha\beta,G} - J^{\|}_{\beta\alpha,H} \right\rangle_{\vec{v}} = 0}$$

Energy

$$m_\alpha \left\{ \left\langle v^2, C_{\alpha\beta} \right\rangle_{\vec{v}} \right\} = -m_\beta \left\{ \left\langle v^2, C_{\beta\alpha} \right\rangle_{\vec{v}} \right\} \Rightarrow \boxed{\left\langle \vec{v}, \vec{J}_{\beta\alpha,G} - \vec{J}_{\alpha\beta,H} \right\rangle_{\vec{v}} = 0}$$

2V Rosenbluth-FP collision operator: numerical conservation of energy

- The symmetry to enforce is:

$$\left\langle \vec{v}, \vec{J}_{\beta\alpha,G} - \vec{J}_{\alpha\beta,H} \right\rangle_{\vec{v}} = 0$$

- Due to discretization error:

$$\left\langle \vec{v}, \vec{J}_{\beta\alpha,G} - \vec{J}_{\alpha\beta,H} \right\rangle_{\vec{v}} = \boxed{\mathcal{O}\left(\Delta_v\right)}$$

- Introduce a constraint coefficient:

$$\left\langle \vec{v}, \boxed{\gamma_{\beta\alpha}} \vec{J}_{\beta\alpha,G} - \vec{J}_{\alpha\beta,H} \right\rangle_{\vec{v}} = 0 \qquad \gamma_{\beta\alpha} = \frac{\left\langle \vec{v}, \vec{J}_{\alpha\beta,H} \right\rangle_{\vec{v}}}{\left\langle \vec{v}, \vec{J}_{\beta\alpha,G} \right\rangle_{\vec{v}}} = 1 + \boxed{\mathcal{O}\left(\Delta_v\right)}$$

$$C_{\alpha\beta} = \Gamma_{\alpha\beta} \nabla_v \cdot \left[\boxed{\gamma_{\alpha\beta}} \vec{J}_{\alpha\beta,G} - \frac{m_\alpha}{m_\beta} \vec{J}_{\alpha\beta,H} \right]$$

2V Rosenbluth-FP collision operator: numerical conservation of momentum+energy

- Simultaneous conservation of momentum and energy:

$$\boxed{C_{\alpha\beta} = \Gamma_{\alpha\beta} \nabla_v \cdot \left[\underline{\underline{\eta}}_{\alpha\beta} \cdot \vec{J}_{\alpha\beta,G} - \frac{m_\alpha}{m_\beta} \vec{J}_{\alpha\beta,H} \right]}$$

with:

$$\underline{\underline{\eta}}_{\alpha\beta} = \begin{bmatrix} \gamma_{\alpha\beta} + \epsilon_{||,\alpha\beta} & 0 \\ 0 & \gamma_{\alpha\beta} \end{bmatrix}$$

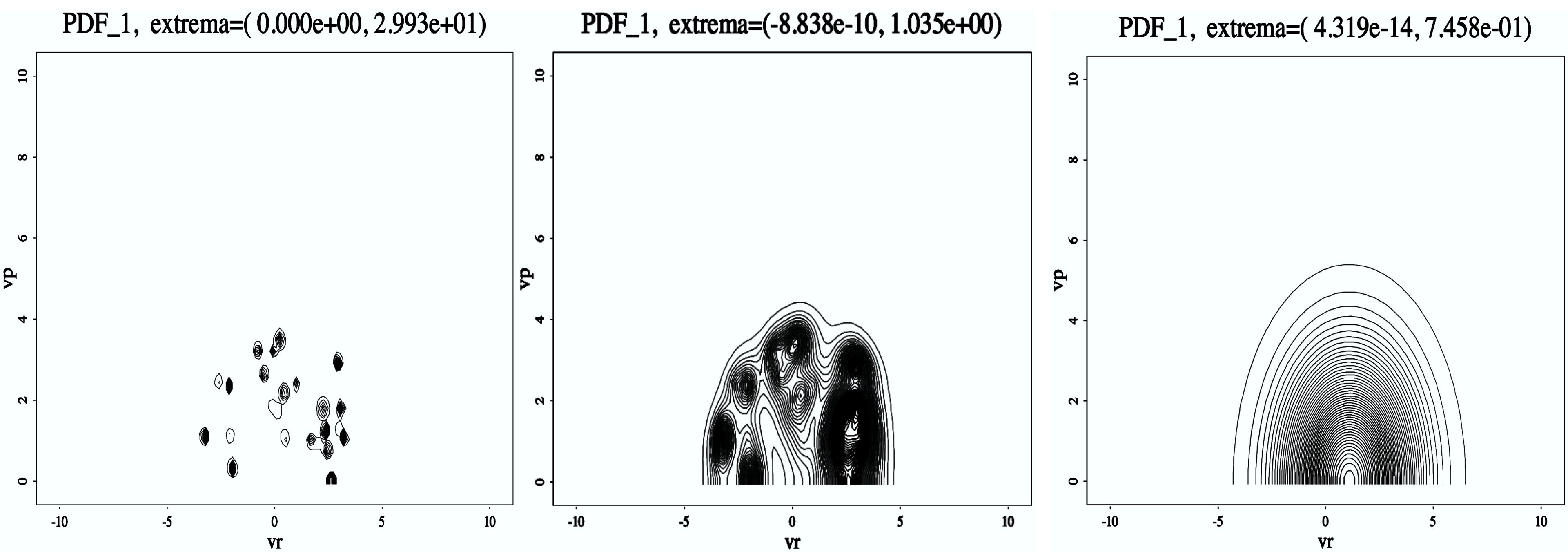
Momentum

Energy

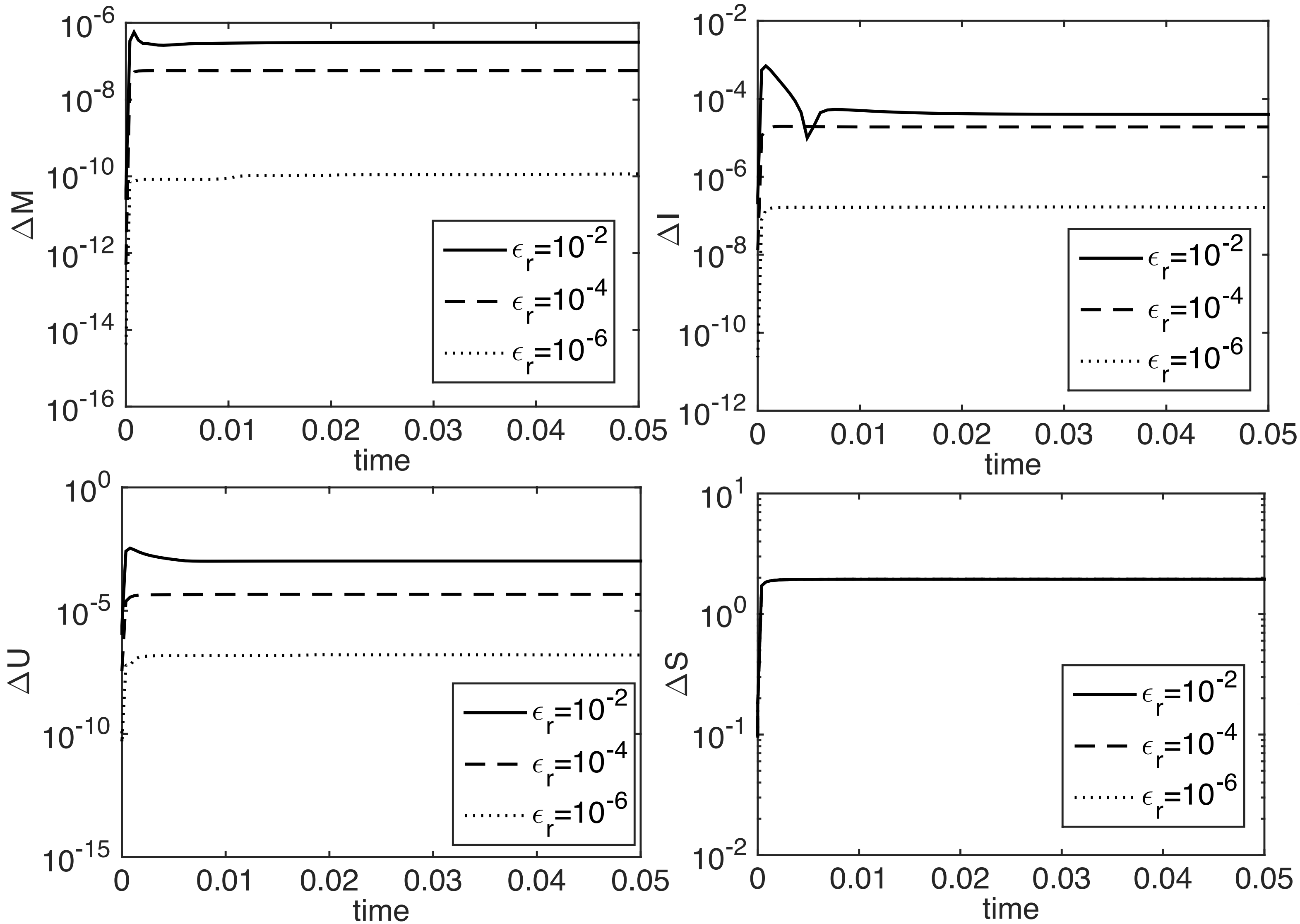
$$\gamma_{\alpha\beta} = \frac{\left\langle \vec{v}, \vec{J}_{H,\beta\alpha} \right\rangle_{\vec{v}} - \epsilon^{+}_{\alpha\beta,||} \left\langle \vec{v}, \vec{J}_{G,\alpha\beta} \right\rangle^{+\infty}_{\vec{v}-\vec{u}}}{\left\langle \vec{v}, \vec{J}_{G,\alpha\beta} \right\rangle_{\vec{v}}}$$

$$\epsilon_{\alpha\beta} = \left\{ \begin{array}{cc} \epsilon^{-}_{||,\alpha\beta} = 0 & \text{if } v_{||} - u_{avg,||,\alpha\beta} \leq 0 \\ \epsilon^{+}_{||,\alpha\beta} = \frac{\left\langle 1, J_{H,\beta\alpha,||} \right\rangle_{\vec{v}} - \gamma_{\alpha\beta} \left\langle 1, J_{G,\alpha\beta,||} \right\rangle_{\vec{v}}}{\left\langle 1, J_{G,\alpha\beta,||} \right\rangle^{+\infty}_{\vec{v}-\vec{u}_{avg,\alpha\beta}}} & \text{else} \end{array} \right\}$$

Numerical Results: Single-species initial random distribution thermalizes to a Maxwellian



Numerical Results: Conservation properties enforced down to nonlinear convergence tolerance



Vlasov equation: Inertial term simultaneous conservation of mass, momentum, and energy

FP equation with adaptivity in velocity space: Temporal inertial terms

- Focus on temporal inertial terms due to normalization wrt $v_{th}(r,t)$ (OD):

$$\boxed{v_{th,\alpha}^2 \frac{\partial \widehat{f}_\alpha}{\partial t} - \frac{\partial_t v_{th,\alpha}^2}{2} \widehat{\nabla}_v \cdot \left(\widehat{\vec{v}} \widehat{f}_\alpha \right) = 0}$$

- Mass conservation can be trivially shown by 0th velocity space moment:

$$v_{th}^2 \frac{\partial n_\alpha}{\partial t} = 0$$

Find symmetry in continuum and enforce via using discrete nonlinear constraints (similar to collisions)

$$\boxed{v_{th,\alpha}^2 \frac{\partial \widehat{f}_\alpha}{\partial t} - \frac{\partial_t v_{th,\alpha}^2}{2} \widehat{\nabla}_v \cdot \left(\vec{\widehat{v}} \widehat{f}_\alpha \right) = 0}$$

Rewrite as:

$$\partial_t \left(v_{th,\alpha}^2 \widehat{f}_\alpha \right) - \partial_t v_{th,\alpha}^2 \left[\boxed{\widehat{f}_\alpha + \frac{\widehat{\nabla}_v}{2} \cdot \left(\vec{\widehat{v}} \widehat{f}_\alpha \right)} \right] = 0$$

Energy conservation shown from 2nd velocity moment:

$$\frac{\partial U_\alpha}{\partial t} = 0$$

This property relies on: $\boxed{\left\langle \widehat{v}^2, \widehat{f}_\alpha + \frac{1}{2} \widehat{\nabla}_v \cdot \left(\vec{\widehat{v}} \widehat{f}_\alpha \right) \right\rangle_{\vec{v}} = 0}$

This property must be enforced numerically:

$$\left\langle \widehat{v}^2, \widehat{f}_\alpha + \frac{\gamma_{t,\alpha}}{2} \widehat{\nabla}_v \cdot \left(\vec{\widehat{v}} \widehat{f}_\alpha \right) \right\rangle_{\vec{v}} = 0 \qquad \gamma_{t,\alpha} = - \frac{\left\langle \frac{\widehat{v}^2}{2}, \widehat{f}_\alpha \right\rangle_{\widehat{v}}}{\left\langle \frac{\widehat{v}^2}{2}, \frac{1}{2} \widehat{\nabla}_v \cdot \left(\vec{\widehat{v}} \widehat{f}_\alpha \right) \right\rangle_{\widehat{v}}}$$

All conservation law can be enforced via recursive application of chain rule

- Rewrite as:

$$\boxed{v_{th,\alpha}^2 \frac{\partial \widehat{f}_\alpha}{\partial t} - \frac{\partial_t v_{th,\alpha}^2}{2} \widehat{\nabla}_v \cdot \left(\widehat{\vec{v}} \widehat{f}_\alpha \right) = 0}$$

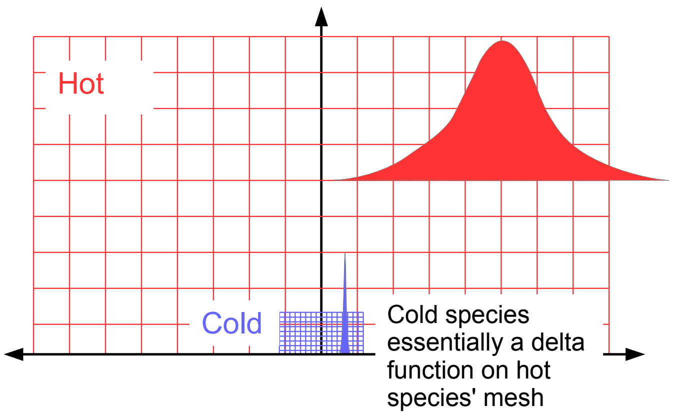
Truncation error

$$\partial_t \left(v_{th,\alpha}^2 \widehat{f}_\alpha \right) - \partial_t v_{th,\alpha}^2 \left[\widehat{f}_\alpha + \gamma_{t,\alpha} \widehat{\nabla}_v \cdot \left(\widehat{\vec{v}} \widehat{f}_\alpha \right) \right] + \xi_{t,\alpha} = 0$$

$$\xi_{t,\alpha} = v_{th,\alpha} \left\{ \partial_t \left(v_{th,\alpha} \widehat{f}_\alpha \right) - \partial_t v_{th,\alpha} \left[\widehat{f}_\alpha + \widehat{\nabla}_v \cdot \left(\underline{\underline{\Upsilon}}_{t,\alpha} \widehat{\vec{v}} \widehat{f}_\alpha \right) \right] \right\} + \eta_{t,\alpha}$$
$$- \left\{ \partial_t \left(v_{th,\alpha}^2 \widehat{f}_\alpha \right) - \partial_t v_{th,\alpha}^2 \left[\widehat{f}_\alpha + \frac{\widehat{\nabla}_v}{2} \cdot \left(\widehat{\vec{v}} \widehat{f}_\alpha \right) \right] \right\}$$

$$\eta_{t,\alpha}(v) = \left\{ v_{th,\alpha}^2 \partial_t \widehat{f}_\alpha - \partial_t v_{th,\alpha}^2 \widehat{\nabla}_v \cdot \left(\widehat{\vec{v}} \widehat{f}_\alpha \right) \right\}$$
$$- v_{th,\alpha} \left\{ \partial_t \left(v_{th,\alpha} \widehat{f}_\alpha \right) - \partial_t v_{th,\alpha} \left[\widehat{f}_\alpha + \widehat{\nabla}_v \cdot \left(\widehat{\vec{v}} \widehat{f}_\alpha \right) \right] \right\}$$

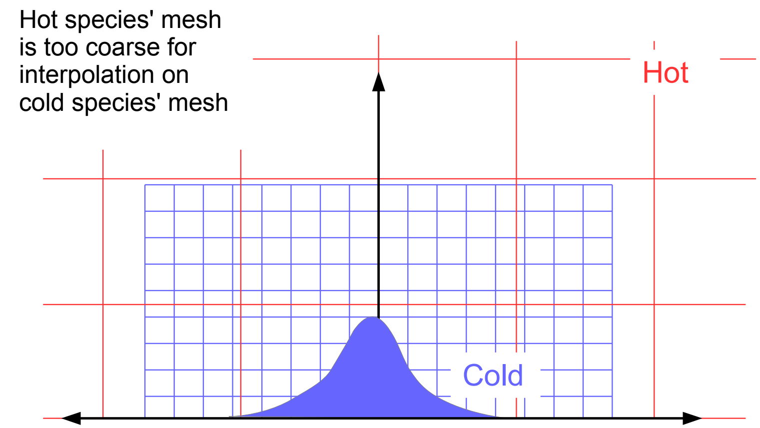
Asymptotic Formulation of Interspecies Collisions for $v_{th,f} >> v_{th,s}$



Argument of exp: $v_f/v_{th,s} >> 1$

$$H_s = \frac{n_s}{v} + \frac{n_s \boldsymbol{V}_s \cdot \boldsymbol{v}}{v^3} + \cdots$$

$$G_s = n_s v - \frac{n_s \boldsymbol{V}_s \cdot \boldsymbol{v}}{v} + \boldsymbol{\nabla}_v \boldsymbol{\nabla}_v v : \left(\frac{1}{2} \int \mathrm{d}^3 v' \, f_s' \boldsymbol{v}' \boldsymbol{v}' \right) + \cdots$$



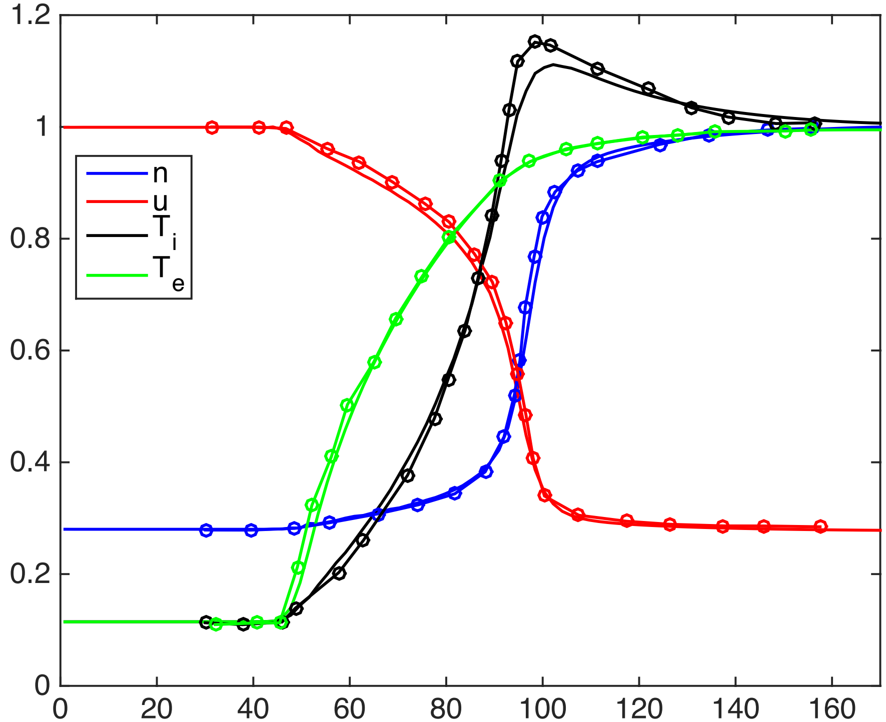
Argument of exp: $v_s/v_{th,f} << 1$

$$H_f = \boldsymbol{v} \cdot \left(\int \mathrm{d}^3 v' \, f_f' \frac{\boldsymbol{v}'}{v'^3} \right) + \frac{1}{2} \boldsymbol{v}\boldsymbol{v} : \left[\int \mathrm{d}^3 v' \, f_f' \boldsymbol{\nabla}_{v'} \boldsymbol{\nabla}_{v'} \left(\frac{1}{v'} \right) \right] - \frac{1}{6} \boldsymbol{v}\boldsymbol{v}\boldsymbol{v} \vdots \left[\int \mathrm{d}^3 v' \, f_f' \boldsymbol{\nabla}_{v'} \boldsymbol{\nabla}_{v'} \boldsymbol{\nabla}_{v'} \left(\frac{1}{v'} \right) \right] + \frac{1}{24} \boldsymbol{v}\boldsymbol{v}\boldsymbol{v}\boldsymbol{v} :: \left[\int \mathrm{d}^3 v' \, f_f' \boldsymbol{\nabla}_{v'} \boldsymbol{\nabla}_{v'} \boldsymbol{\nabla}_{v'} \boldsymbol{\nabla}_{v'} \left(\frac{1}{v'} \right) \right] + \cdots$$

$$G_f = \frac{1}{2} \boldsymbol{v}\boldsymbol{v} : \left(\int \mathrm{d}^3 v' \, f_f' \boldsymbol{\nabla}_{v'} \boldsymbol{\nabla}_{v'} v' \right) - \frac{1}{6} \boldsymbol{v}\boldsymbol{v}\boldsymbol{v} \vdots \left(\int \mathrm{d}^3 v' \, f_f' \boldsymbol{\nabla}_{v'} \boldsymbol{\nabla}_{v'} \boldsymbol{\nabla}_{v'} v' \right) + \frac{1}{24} \boldsymbol{v}\boldsymbol{v}\boldsymbol{v}\boldsymbol{v} :: \left(\int \mathrm{d}^3 v' \, f_f' \boldsymbol{\nabla}_{v'} \boldsymbol{\nabla}_{v'} \boldsymbol{\nabla}_{v'} \boldsymbol{\nabla}_{v'} v' \right) + \cdots$$

[5] W.T. Taitano, JCP accepted (2016)

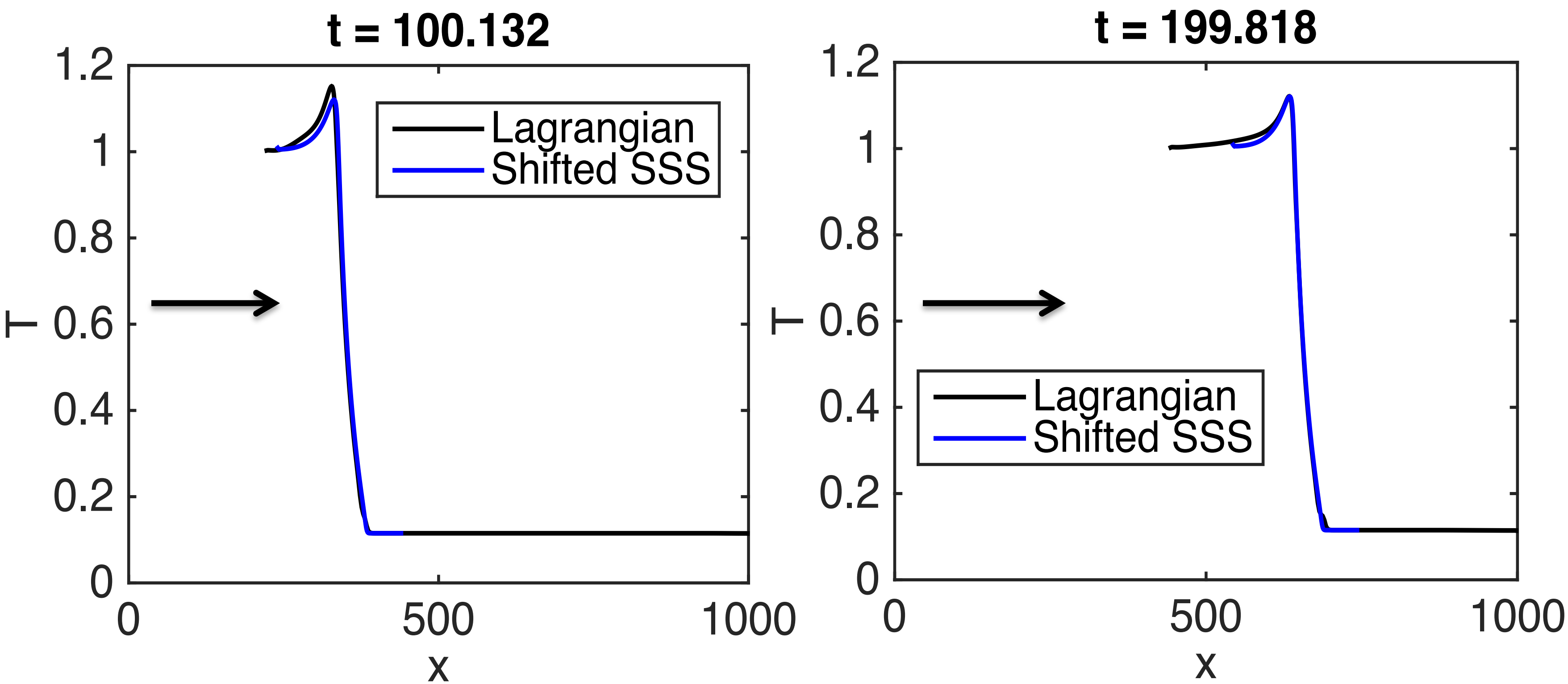
1D2V Mach 5 shock agrees well with known reference solution



M=5 planar steady state shock solution (SSS) comparison between iFP (solid line) and reference solution from [10] (open circles).

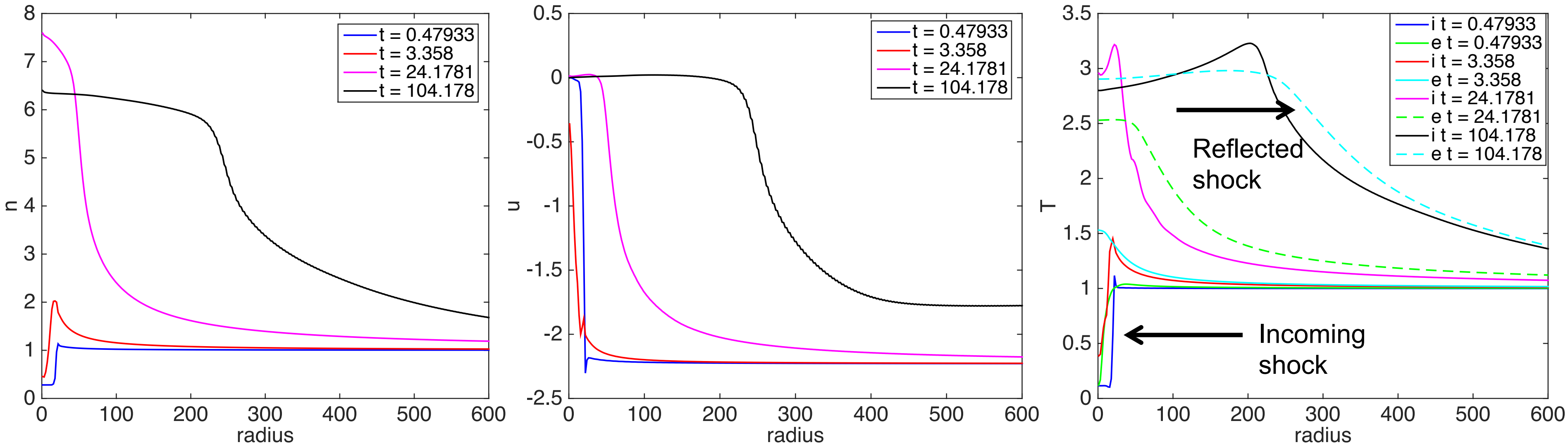
[10] F. Vidal et al., PoF B, 3182 (1993)

Lagrangian mesh tracks shock



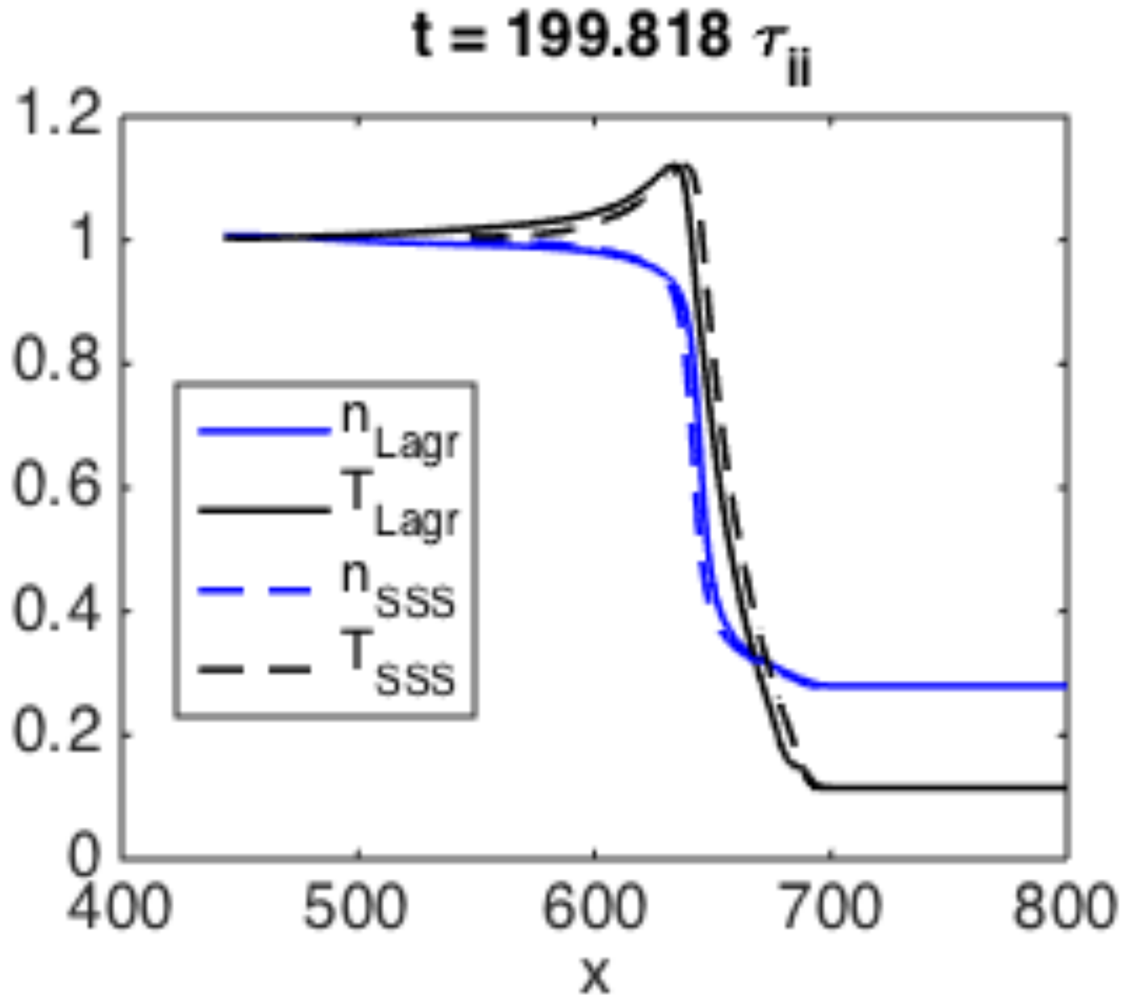
Test of Lagrangian mesh capability for a M=5 shock in lab frame. A good agreement in solutions between Lagrangian mesh and SSS is achieved.

Spherical geometry is being tested

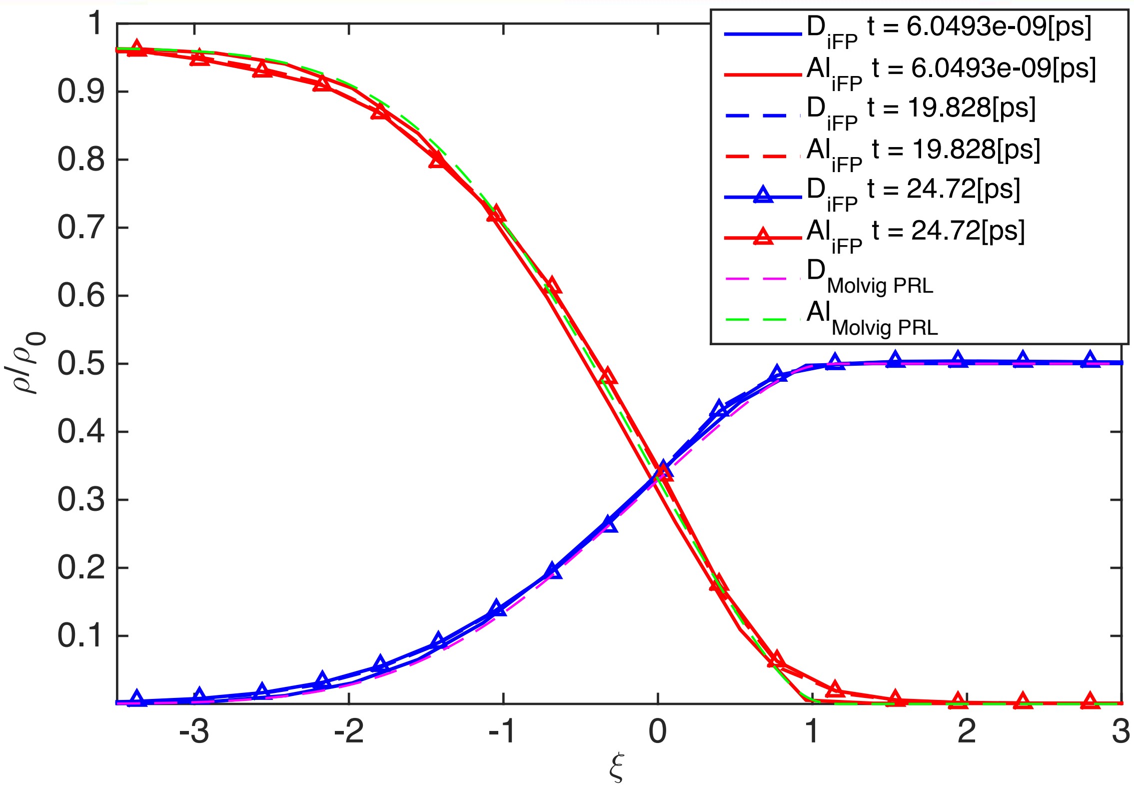


Test of spherical shock convergence. Shock reflection is observed.

More moments for Lagrangian mesh

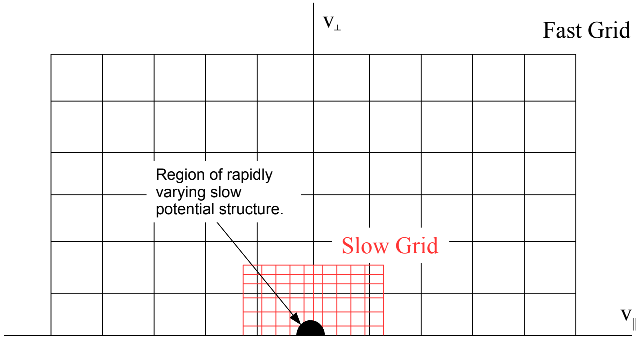


Stably and accurately integrate with $\Delta t >> \tau_{col}$



Test of implicit solver with D-Al interface problem with $\Delta t = 4\text{x}10^4\ \tau_{col}$.

Velocity space adaption does not help for interspecies collisions



- For electron-ion collisions, $v_{th,e}/v_{th,i} >> 1$
- Similarly, for α-ion collisions, $v_{th,\alpha}/v_{th,I} >> 1$
- Very stringent mesh resolution requirements if determining potentials via:

$$\nabla_v^2 H_j(\vec{v}) = -8\pi f_j(\vec{v}) \qquad \nabla_v^2 G_j(\vec{v}) = H_j(\vec{v})$$

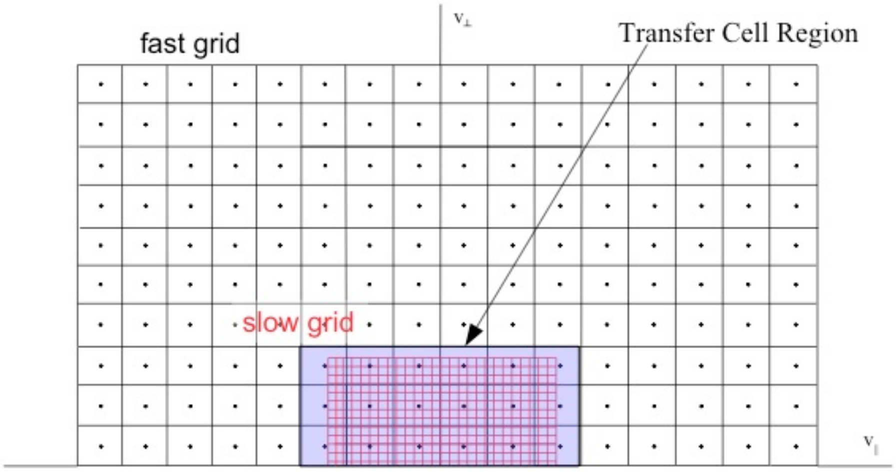
- Mesh requirement grows as:

$$N_v^d \propto \left(\frac{v_{th,f}}{v_{th,s}}\right)^d$$

- Velocity space adaption helps **ONLY** for self-species, but not for interspecies! We need asymptotics

Asymptotics: Fast on slow

- Asymptotic potentials diverge as v → 0
- Solution: Near v = 0, we **coarse-grain** slow potentials to modify singularity

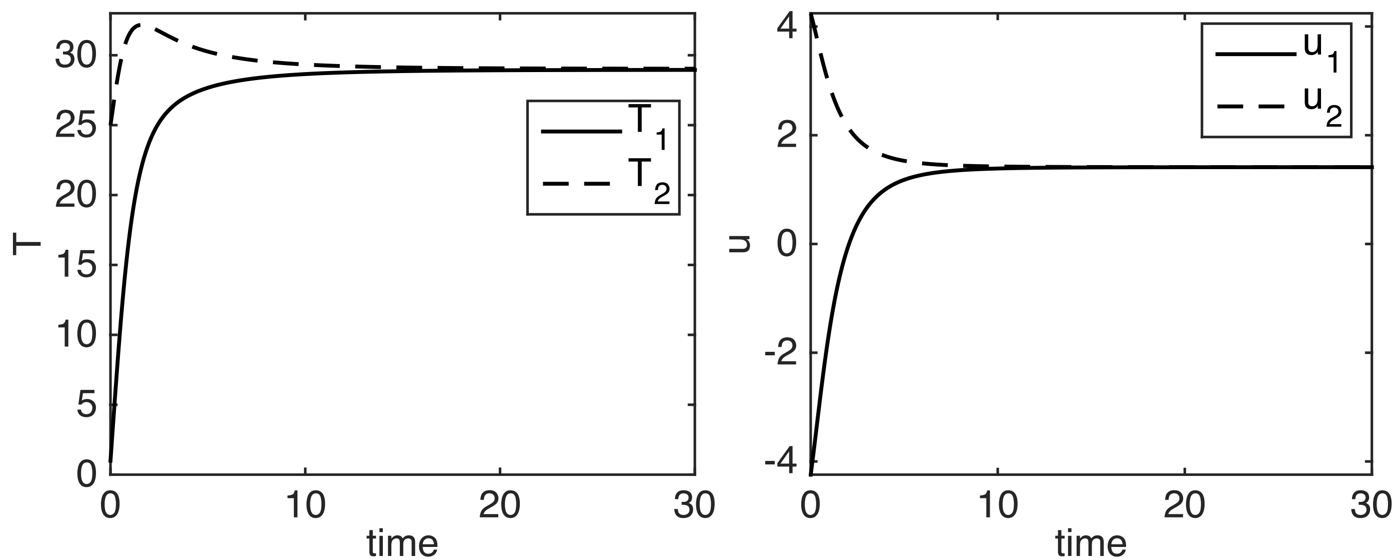


$$H_{fs} = \left\{ \begin{array}{cc} H_{fs,asy} & \text{if } \vec{v}_f \notin \Omega_{TCR} \\ \langle H_{ss} \rangle_{\Omega_{TCR}} & \text{else} \end{array} \right\}$$

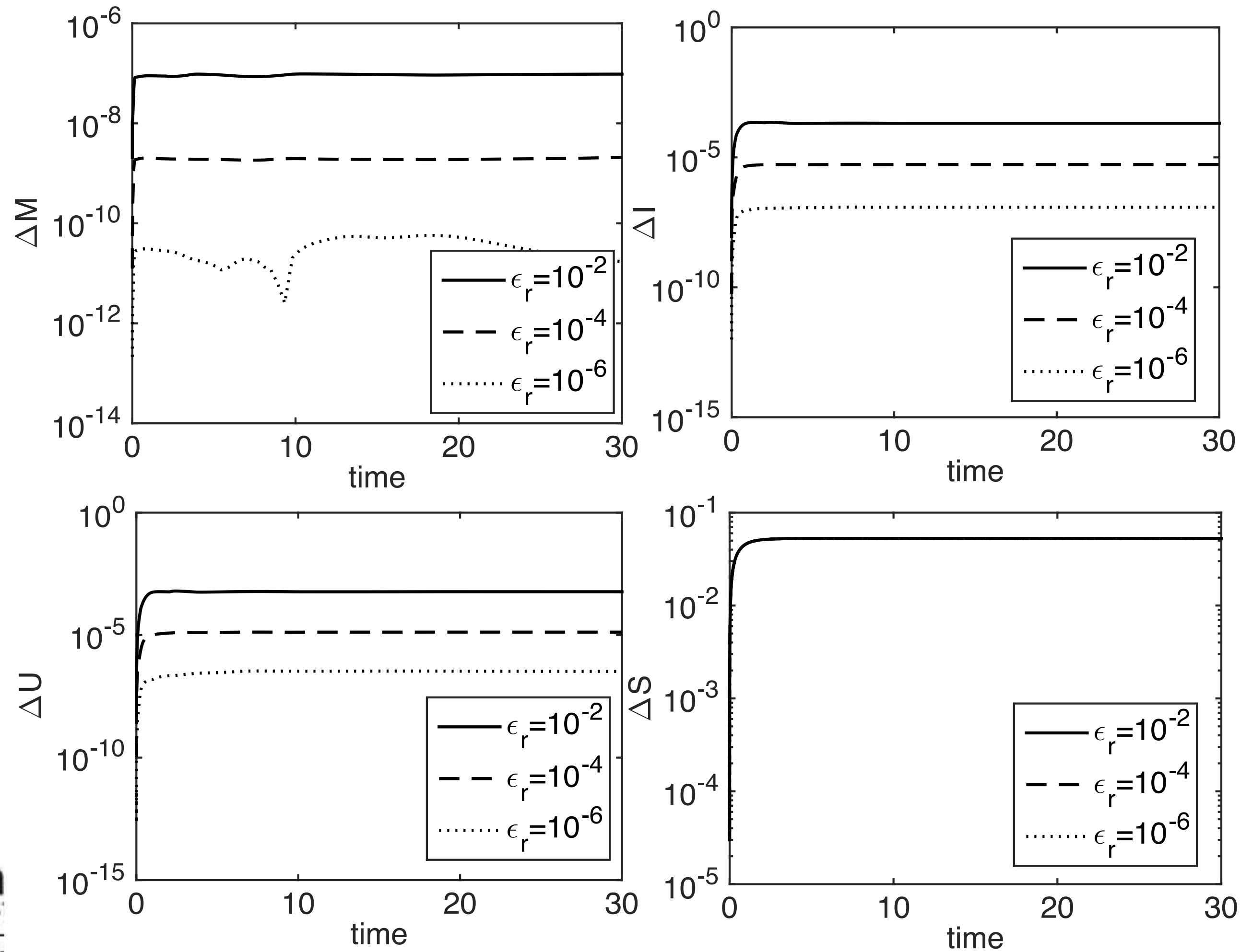
$$\langle H_{ss} \rangle_{\Omega_{TCR}} = \frac{\int_{\Omega_{TCR}} H_{ss} d^3 v}{\int_{\Omega_{TCR}} d^3 v}$$

$$\nabla_v^2 G_{fs} = H_{fs}$$

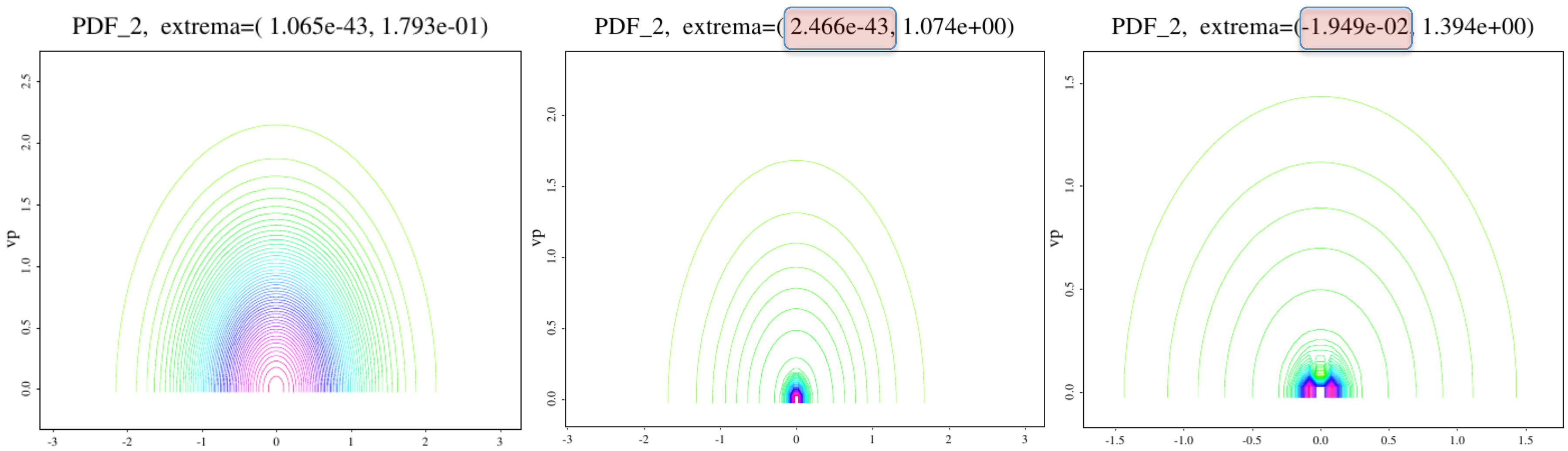
Numerical Results:
Two-species thermal and momentum equilibration



Numerical Results: Conservation is enforced down to nonlinear tolerance



Non-Maxwellian effects for hot-cold proton thermalization



Initial Condition

With positivity

Without positivity

Our approach: nonlinearly implicit, adaptive, conserving Rosenbluth-VFP (cont.)

- Why Rosenbluth-VFP?
- Linearization and/or the use of asymptotic approximations of collision operators are not warranted in these systems:
  - Linearization is not allowed because deviations from Maxwellian can be significant (Kn ~ 0.1 in fuel, boundary effects at material boundaries)
  - Ion thermal velocities are comparable to Gamow peak at bang time ($v_{th}/v_G \sim 1/\sqrt{3}$)
  - Multiple ion species with similar mass and temperatures
- Nonlinear Rosenbluth-VFP allows for first-principles simulations

Static uniform mesh is not practical

- Temperature disparities of 10^4 (for a single species)

$$v_{th}^{max}/v_{th}^{min} \sim 100$$

- 10 points per v_{th} $\Rightarrow \Delta v \sim v_{th}^{min}/10$

$$N_v \sim (v_{th}^{max}/\Delta v)^2 \sim 10^6$$

- For multiple species (e.g. alpha-D/T)

$$N_v^* \sim N_v 30^2 \sim 10^9$$

- Static spatial resolution:

$$N_r \sim 10^3 - 10^4$$

$$\boxed{N \sim N_v^* \times N_r \sim 10^{12} - 10^{13}}$$

Challenges of Rosenbluth-VFP: temporal stiffness. Explicit method are impractical

- Collision frequency dictates explicit time step:

$$\Delta t_{exp}^{coll} \sim \frac{\Delta v^2}{D} \sim \frac{\Delta v^2}{v_{th}^2 \nu_{coll}}$$

- Typical conditions at end of compression phase:

$$\boxed{\Delta t_{exp}^{coll} \sim \frac{1}{10}\left(\frac{\Delta v}{v_{th}^{min}}\right)^2 \nu_{coll}^{-1} \sim 10^{-9}\, ns}$$

$$\boxed{N_{\Delta t} \sim 10^{10}}$$

Our approach: nonlinearly implicit, adaptive, conserving Rosenbluth-VFP

- Adaptive meshing to alleviate mesh requirements:
  - Velocity space adaptivity via renormalization (N_v~10^4-10^5)

$$\hat{v} = v/v_{th}(r,t)$$

  - Spatial adaptivity via Lagrangian mesh ($N_r \sim 10^2$)

$$\boxed{N = N_v \times N_r \sim 10^6 - 10^7}$$

- Strict conservation properties (mass, momentum, energy).

Logo choices

OR